EXPLORING CONFORMATIONAL SPACES AND AGGREGATION PREFERENCES OF SERINE-ASPARAGINE AND VALINE-ASPARAGINE DIMERS BY IRMPD SPECTROSCOPY AND QUANTUM CHEMISTRY

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Amino acids, often refered as the building blocks of proteins, are not only crutial in our body for all sorts of biological functions they support, but also are significantly important to chemistry and life sciences for their chirality properties. The mirror-imaged pair of a chiral amino acid share the same chemical formula but may respond very differently when interacting with a chiral acceptor site. In this presented work, the protonated dimers of asparagine with either serine or valine in their homochiral and heterochiral forms were investigated using an Infrared Multiple-Photon Dissociation (IRMPD) spectrometer. A three-tiered approach was developd to identify possible homochiral and heterochiral dimers. Harmonic frequency calculations were further carried out to interpret the observed IRMPD spectra. Analyses of these ensembles reveal a strong preference for the migration of the excess proton during the photodissociation process from serine and valine to asparagine. The structural and energetic relationships in the protonated homochiral and heterochiral serine-asparagine and valine-asparagine dimers will also be discussed in this talk.

1. M. Heger, J. Cheramy, F. Xie, Z. Chen and Y. Xu, J. Mol. Spectrosc., 2018, 352, 36–44.